Week 1 Notes

Lecture 1 & 2

1 Supervised Learning (lecture 1)

Def: *model*; a model is some structure that uses parameters to perform a function. An example of a model is $y = wx + b$, which is a linear model. Technically speaking, we should write a linear model as (refer to 1.1 for more info):

$$\hat{y} = \sum_{j=1}^{m} w_j \cdot X_j + b = XW^T + b$$

where we have a weight, w_j for each feature X_j, with a bias term, b, and an output vector $\hat{y}$. The intuition is that, the parameters (i.e. W and b) can be changed based off the data so that the model performs the optimal function/prediction/output. We say that the model learns because it is able learn the right combination of W and b to give an optimal output (global optimal is not guraneed; more info next lecture). The weights, w_j, determines how important a feature x_j is to the optimal solution of $\hat{y}$. We can think of a machine learning model as a mathematical function, F, with 1 or more features likeso:

$$\hat{y} = F(X_1, ..., X_m) = w_1 X_1 + ... + w_m X_m + b$$

For example, the inputs of a weather model can be the humidity, temperature, air speed, etc. And the output could be how much it will rain (*regression model*) or a probability distributon of what the weather will be like (*classification model*). In a regression model the output $y \in \mathbb{R}$ while the output of a classification model is a probability distribution $Y \sim p(x)$. A classification model with 2 classes is a binary classification model, a model with more than 2 classes is a multi-class classificatiton model.

Def: *supervised learning*; when we can train a model with labeled data. For example, given an image of a dog the label will be "dog". Formally, we can express this as:

$$D = \{(x_1, y_1), ..., (x_n, y_n)\}$$

where D represents our dataset, x_i is the input vector to the i^{th} sample and y_i is the corresponding label to the i^{th} sample. Note that, we call x_i the input vector because we can only pass in numbers. For example, an RGB image would be a matrix of size $(H \times W \times 3)$. Similarly, the output has to be a vector and cannot be something like the label "dog". We need encode the label using a technique such as *one-hot encoding* for categorical data or Universal Sentence Encoder (USE) for sentences in NLP. Ultimately, our goal in supervised learning is to learn a function F such that for a new pair of data (x, y), we have $F(x) \approx y$ with high probability.

1.1 Linear Models and Why $\hat{y} = XW^T + b$?

Naively, we can implement a linear model using the algorithm:

Algorithm 1 Naive Linear Model

```
1: $y = b$
2: **for** $j$ in range($m$) **do**
3:     $y$ += $w_j * x_j$                ▷ simple scalar multiplication
4: **end for**
```

However, this is a very ugly implementation and For-loops in Python are slow. Instead, we want to express them in terms of matrices. Generally we want X to have shape $(n \times m)$ where n is the number of data and m is the number of features (i.e each row/data has m features), therefore a $(m \times n)$ shape would not make sense. We also want the output to have shape $(n \times p)$ where p are the predictions (i.e. each row/data has p predictions). The problem with $W^T X$ is that we need to transpose the X matrice which does not make sense to do so:

$$(?, ?) \times (n, m) \rightarrow (n, p)$$

Instead, writing it as XW^T makes more sense:

$$(n, m) \times (?, ?) \rightarrow (n, p)$$

where, the weight matrice can now have shape (m, p). However, we want to represent the weight matrice as shape (p, m) as it is equivalent to saying "a prediction p can be made if given m features". Therefore, the dimensions of X, W, and output will be:

- $W \rightarrow (p, m)$
- $X \rightarrow (n, m)$
- Out $\rightarrow (n, p)$

We can see this convention being adopted by Pytroch (torch.nn.Linear)[1]. Another reason why we want to represent W and X as matrices is because it's easier to differentiate (for gradient descent).

2 Regression (lecture 1)

2.1 Linear Regression

If we have a linear model (i.e. $y = XW^T + b$) finding the particular parameters (W and b) for this linear function is called linear regression. We can think of linear regression as the line of best fit.

3 Loss Function (lecture 2)

Def: *loss function*; measures how *poor* the model is performing. The lower the loss, the better. A loss of zero means it makes perfect predictions. An example of a well-known loss function is the *Mean Absolute Error (MAE)* and can be written formally as:

$$\text{MAE}(y, \hat{y}') = \frac{1}{N} \sum_{n}^{N} y_n - \hat{y}'_n$$

where y_n is the n^{th} label in the data and $\hat{y}'_n$ is the output of the model when given the n^{th} data, x_n. Another loss function is the *Mean Square Error (MSE)* and can be written formally as:

$$\text{MSE}(y, \hat{y}') = \frac{1}{N} \sum_{n}^{N} (y_n - \hat{y}'_n)^2$$

The MAE will prefer outliers while MSE will prefer none to be extremely far. It is common practice to normalize the loss by the total number of training samples, n, so that the output can be interpreted as the average loss per sample [Cornell CS4780, Lecture 1, Fall 2018].

[1]https://pytorch.org/docs/master/generated/torch.nn.Linear.html

3.1 Properties of the Loss Function

1. The minimal loss value should correspond to the line of best fit
2. The loss must be defined for all outputs and labels (no divide by 0)
3. The loss function should be differentiable (for gradient descent)

Therefore, a loss function, $\ell(w)$, is convex, continuous, and differentiable.

4 Gradient Descent (lecture 2)

Gradient of loss, ∇Loss, is the *direction of steepest ascent*. The negative gradient of loss, $-\nabla$Loss, is the direction of steepest descent. The gradient of loss with respect to the weight can be written as:

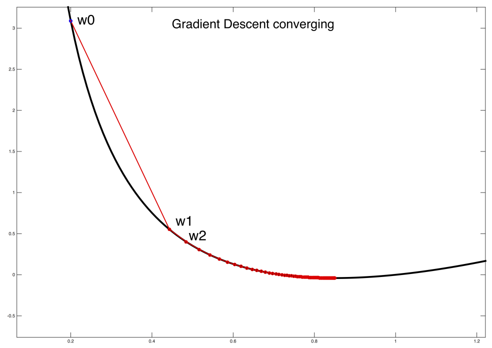
$$\nabla_W \text{Loss} = \frac{\partial L}{\partial W} = \left(\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}, ..., \frac{\partial L}{\partial W_m}\right)$$

The intuition behind the gradient descent algorithm is to iteratively update W_i in the direction of the negative gradient (steepest descent) until we reach the optimal solution. Taking a small enough step, α, in the negative gradient is guranteed to reduce loss and convergence to an optimal model. The step size, α, is also known as the *learning rate* is a hyperparameter. Formally, we can write all of this as:

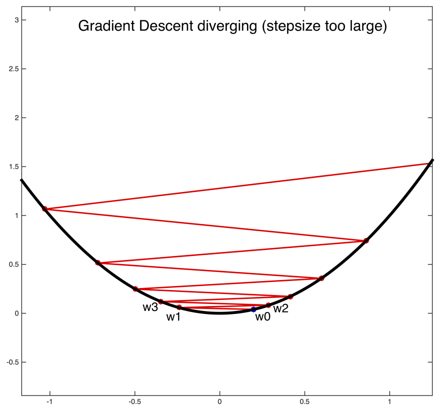
$$W = W - \alpha \nabla_W \text{Loss}$$

$$W_i = W_i - \alpha \frac{\partial L}{\partial W_i}$$

Whether we converge to an optimal solution depends on how we set the learning rate α. The model is unable to converge if α is too large, and is unable/expensive to converge because α is too small. Usually $\alpha > 0$ and is some small number. We say the model converges when we see that $\frac{\partial L}{\partial w_i}$ is minimized ($= 0$) or does not change after each iteration of the gradient descent algorithm[2].



(a) α is just right



(b) α is too large

Figure 1: Consequence of choosing α, [Cornell CS4780, Lecture 7, Fall 2018]

[2]Assume that this model has no bias (i.e. $b = 0$) for simplicity